**PREDICTING FLUID COMPOSITIONS AND MINERAL ALTERATION AROUND NUCLEAR WASTE EMPLACEMENT TUNNELS.** N. Spycher<sup>1</sup>, E. Sonnenthal<sup>1</sup>, and J. Apps<sup>1</sup>, <sup>1</sup>Lawrence Berkeley National Laboratory, MS 90-1116, 1 Cyclotron Road, Berkeley, California 94720 (nspycher@lbl.gov).

Introduction: This study investigates coupled thermal, hydrological, and chemical processes that could take place around waste-emplacement tunnels (drifts) at the potential high-level nuclear waste repository at Yucca Mountain, Nevada. Upon heating as a result of waste decay, water held in the unsaturated rock matrix boils and travels as vapor in fractures. In cooler regions, it condenses and may drain back towards boiling zones. Knowing whether such continuous boiling and refluxing alters the rock fracture permeability around drifts is important for repository design. Also, the composition of fluids (water and gas) that could enter the drifts needs to be evaluated to aid in the design of corrosion-resistant waste canisters.

Approach: Numerical simulations were performed considering water, vapor, air, and heat transport; reactive gas, mineral, and aqueous phases; porosity-permeability-capillary pressure coupling; and dual permeability (fractures and rock matrix). This was achieved by enhancing the multicomponent reactive transport model TOUGHREACT [1] to handle high-temperature, boiling environments. Two-dimensional vertical and symmetrical half-drift models that incorporate hydrogeologic data from field studies were developed for various scenarios, including possible climate changes and different drift designs, geochemical systems, and geologic representations [2].

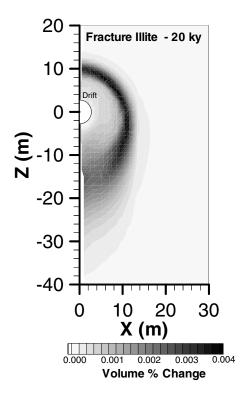
Results: After waste emplacement, rock around the drift dries out. The drift crown reaches temperatures near 150°C, then eventually cools and rewets after 1,000 to 2,000 years through natural infiltration. Temperature returns to ambient values in 100,000 years. Over this entire period, predicted trends in fluid compositions and mineral alteration around drifts do not vary significantly between evaluated scenarios. These trends are controlled by various coupled mechanisms. Upon heating and boiling, CO2 exsolution from pore waters drives pH up and causes calcite precipitation. However, in condensation zones, pH generally decreases resulting from dissolution of CO2 mobilized with steam, causing calcite dissolution and enhancing feldspar alteration to clays (Figure 1). Heat also enhances silica dissolution from wallrock minerals and possibly zeolite alteration. Other minerals (gypsum and fluorite) also precipitate by evaporative concentration.

Upon cooling, amorphous silica precipitates. During later cooling stages, calcite also precipitates when infiltration waters replenished in aqueous carbonate warm up as they percolate from the ground surface towards the drift (where temperatures remain above

ambient values for thousands of years). Amorphous silica and calcite account for essentially all the predicted fracture porosity decrease around the drift (< 3%). During rewetting of fractures at the drift crown, neutral to moderately alkaline pH values are predicted, with water salinity typically remaining less than a few thousand mg/l.

Significance of Findings: The small calculated porosity change has a negligible effect on the fracture rock permeability and flow patterns around drifts. This conclusion is controversial in light of other studies suggesting fracture sealing could occur. The predicted dilute to moderate water salinity and mildly alkaline pH have been used as concentration bounds for assessing the performance of waste canisters and other in-drift engineered systems. More work is underway to reduce the uncertainty of the model and evaluate how this uncertainty affects the conclusions drawn here.

**References:** [1] Xu T. and Pruess K. (2001) *AJS* (*in press*). [2] Sonnenthal E. and Spycher N. (2000) Lawrence Berkeley National Laboratory, Report LBID 2340, Berkeley, California.



**Figure 1**. Illite precipitation in fractures. Maximum precipitation occurs in a zone coinciding with the maximum extent of the dryout zone around the drift.